CAS ONLINE PRINTOUT

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(FILE 'HOME' ENTERED AT 12:00:24 ON 02 MAR 2006)

FILE 'REGISTRY' ENTERED AT 12:01:08 ON 02 MAR 2006
L1 STRUCTURE UPLOADED
L2 50 S L1
L3 1321 S L1 FUL
L4 STRUCTURE UPLOADED
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L6 0 SEARCH L5 SSS SUB=L3 FUL
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L8 1321 SEARCH L7 SSS SUB=L3 FUL
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FILE 'CAPLUS' ENTERED AT 12:09:30 ON 02 MAR 2006
L13 33 S L12

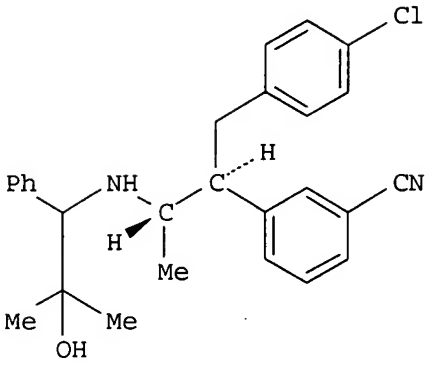
=> d bib abs hitstr 1-33

L13 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:429387 CAPLUS
DN 142:481820
TI Preparation of aralkyl amines as cannabinoid-1 receptor modulators
IN Shah, Shrenik K.; Truong, Quang T.; Qi, Hongbo; Hagmann, William K.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 137 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005044785	A1	20050519	WO 2004-US35846	20041027
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 2003-515705P	P	20031030		

OS MARPAT 142:481820
GI

CAS ONLINE PRINTOUT



I

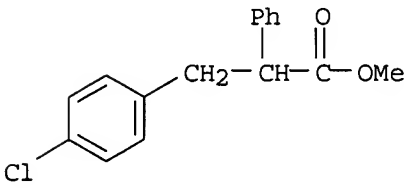
AB Aralkyl amines ((Ar1X)C(R1)(Ar2)CH(R2)N(R3)C(R4)(R5)Ar3 (I); variables defined below; e.g. 2 diastereomers of 3-[1-(S*)-(4-chlorobenzyl)-2-(S*)-[[2-hydroxy-2-methyl-1-(R*)-phenylpropyl]amino]propyl]benzonitrile (shown as II)) are antagonists and/or inverse agonists of the Cannabinoid-1 (CB1) receptor and are useful in the treatment, prevention and suppression of diseases mediated by the CB1 receptor. The compds. of the present invention are useful as centrally acting drugs in the treatment of psychosis, memory deficits, cognitive disorders, migraine, neuropathy, neuro-inflammatory disorders including multiple sclerosis and Guillain-Barre syndrome and the inflammatory sequelae of viral encephalitis, cerebral vascular accidents, and head trauma, anxiety disorders, stress, epilepsy, Parkinson's disease, movement disorders, and schizophrenia. The compds. are also useful for the treatment of substance abuse disorders, including alc. and nicotine addiction, the treatment of obesity or eating disorders, as well as the treatment of asthma, constipation, chronic intestinal pseudo-obstruction, and cirrhosis of the liver. For I: R1 = H, C1-4alkyl, (un)substituted with 1-3 Re, halogen, and -ORd; R2 = H, C1-4alkyl, and aryl, wherein each alkyl and aryl moiety is (un)substituted with 1-3 Re; R3 = H, and C1-4alkyl, (un)substituted with 1-3 Re; R4 = H, C1-10alkyl, C2-10alkenyl, C2-10alkynyl, C1-10alkyloxycarbonyl-, C3-10cycloalkyl, aryl-C1-6alkyl-, and heteroaryl-C1-6-alkyl-, wherein each alkyl, alkenyl, and alkynyl moiety is (un)substituted with 1-4 Ra and each aryl, heteroaryl, and cycloalkyl moiety is (un)substituted with 1-3 Rb and oxo; R5 = H, and C1-4alkyl, (un)substituted with 1-3 Re. Ar1 = C1-10alkyl, C2-10alkenyl, C2-10alkynyl, C3-10cycloalkyl, cycloheteroalkyl, aryl, and heteroaryl, wherein each alkyl, alkenyl, and alkynyl moiety is (un)substituted with 1-3 Ra, each aryl and heteroaryl moiety is (un)substituted with 1-4 Rb and each cycloalkyl and cycloheteroalkyl moiety is (un)substituted with 1-4 Rb and oxo; Ar2 = -ORd, -CO2Rd, C3-10cycloalkyl, cycloheteroalkyl, aryl, and heteroaryl, wherein each cycloalkyl, cycloheteroalkyl moiety is (un)substituted with 1-4 Rb and oxo and each aryl and heteroaryl moiety is (un)substituted with 1-4 Rb; Ar3 = cycloalkyl, aryl, and heteroaryl, wherein each cycloalkyl, aryl and heteroaryl moiety is (un)substituted with 1-4 Rb; X = a bond, C1-4alkyl, O, S, and -NRc-, provided that when X is O, S, or -NRc-, then R1 is H or C1-4alkyl and Ar2 is not -ORd; addnl. details are given in the claims. Although the methods of preparation are not claimed, >100 example prepns. and/or characterization data for I are included. For example, II was prepared from [3-(4-chlorophenyl)-2-(S*)-(3-cyanophenyl)-1-(S*)-methylpropyl]amine, 2-hydroxy-2-methylpropiophenone and NaHB(OAc)3 in dichloroethane. Compds. I were tested in a CB1 binding assay and found to have an IC50 value of ≤2 μM. Selective CB1 antagonist/inverse agonist compds. have IC50s 100-fold greater in the CB2 binding assay than in the CB1 assay, and generally have IC50s >1μM in the CB2 binding assay. CB1 antagonist/inverse agonist compds. I generally

have EC50s of <1 μM in a CB1 functional assay and selective CB1 antagonist/inverse agonists generally have EC50s >1 μM in the CB2 functional assay.

IT **92907-23-8P**, 3-(4-Chlorophenyl)-2-phenylpropanoic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aralkyl amines as cannabinoid-1 receptor modulators)

RN 92907-23-8 CAPLUS

CN Benzenepropanoic acid, 4-chloro-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:281753 CAPLUS
DN 142:355050
TI Preparation of aryl sulfonamides as cannabinoid CB1 receptor antagonists and/or inverse agonists.
IN Armstrong, Helen M.; Chang, Linda L.; Guthikonda, Ravindra N.; Hagmann, William K.; Lin, Linus S.; Shah, Shrenik K.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 122 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2005027837	A2	20050331	WO 2004-US30122	20040914

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

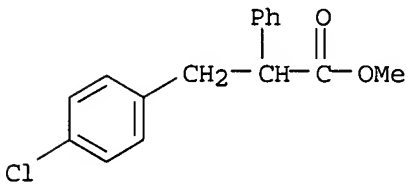
PRAI US 2003-504377P P 20030918
OS MARPAT 142:355050
AB R1R2R6CCR3R7NR4SO2R5 [I; R1 = (substituted) alkyl, cycloalkyl(alkyl), cycloheteroalkyl(alkyl), (hetero)aryl(alkyl), etc.; R2 = (substituted) alkyl, cycloalkyl(alkyl), cycloheteroalkyl(alkyl), (hetero)aryl(alkyl); R3, R7 = H, (substituted) alkyl, cycloalkyl(alkyl), (hetero)aryl(alkyl), cycloheteroalkyl(alkyl); R4 = H, (substituted) alkyl; R5 = (substituted) alkyl, alkenyl, alkynyl, cycloheteroalkyl(alkyl), cycloalkyl(alkyl), (hetero)aryl(alkyl), etc.; R6 = H, OH, alkyl, halo, cyano; with provisos], were prepared Thus, 2-amino-3,4-bis(4-chlorophenyl)butane hydrochloride,

diisopropylethylamine, and tert-butylsulfinyl chloride were stirred together in CH2Cl2 for 2 h to give N-[2,3-bis(4-chlorophenyl)-1-methylpropyl]-2-methyl-2-propanesulfinimide. This was stirred with m-ClC6H4C(O)OOH in CH2Cl2 to give N-[2,3-bis(4-chlorophenyl)-1-methylpropyl]-2-methyl-2-propanesulfonimide. I generally have EC50 values of <1 μM in a CB1 functional assay.

IT **92907-23-8P**, 3-(4-Chlorophenyl)-2-phenylpropanoic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryl sulfonamides as cannabinoid CB1 receptor antagonists and/or inverse agonists)

RN 92907-23-8 CAPLUS

CN Benzenepropanoic acid, 4-chloro-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 3 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:467848 CAPLUS

DN 141:38363

TI Preparation of propanamide derivatives as cannabinoid-1 receptor antagonists

IN Hagmann, William K.; Lin, Linus S.; Shah, Shrenik K.; Guthikonda, Ravindra N.; Qi, Hongbo; Chang, Linda L.; Liu, Ping; Armstrong, Helen M.; Jewell, James P.; Lanza, Thomas J., Jr.

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 99 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004048317	A1	20040610	WO 2003-US7039	20030307
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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	BR 2003008349	A	20050125	BR 2003-8349	20030307
	NO 2004003803	A	20050524	NO 2004-3803	20040910
PRAI	US 2002-428415P	P	20021122		
	WO 2003-US7039	W	20030307		

OS MARPAT 141:38363

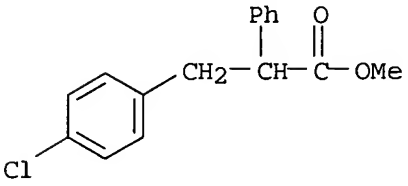
AB The title compds. with general formula of R1R2CH-CH(Me)-NH-CO-C(Me2)-O-R3 [wherein R1 = heterocyclyl, aryl, heteroaryl, (un)substituted amino, etc.; R2 = alkyl, cycloalkylalkyl, arylalkyl, heteroarylalkyl, etc.; R3 =

cycloalkyl, aryl, heteroaryl, etc.] or pharmaceutically acceptable salts thereof are prepared as cannabinoid-1 (CB1) receptor antagonists. For example, N-[2,3-bis(4-chlorophenyl)-1-methylpropyl]-2-(4-chlorophenoxy)-2-methylpropanamide was prepared in a multi-step synthesis. The compds. are useful for the treatment of substance abuse disorders, the treatment of obesity or eating disorders, as well as the treatment of asthma, constipation, chronic intestinal pseudo-obstruction, and cirrhosis of the liver (no data).

IT **92907-23-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of propanamide derivs. as cannabinoid-1 receptor antagonists)

RN 92907-23-8 CAPLUS

CN Benzenepropanoic acid, 4-chloro-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:837028 CAPLUS
DN 139:337785
TI Preparation of substituted arylamides as cannabinoid-1 receptor antagonists and/or inverse agonists for use as psychotropic drugs
IN Hagmann, William K.; Lin, Linus S.; Shah, Shrenik K.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 191 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003087037	A1	20031023	WO 2003-US9800	20030401
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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CA 2480856	AA	20031023	CA 2003-2480856	20030401
AU 2003226149	A1	20031027	AU 2003-226149	20030401
EP 1494997	A1	20050112	EP 2003-746565	20030401
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US 2005154202	A1	20050714	US 2003-509277	20030401
JP 2005527586	T2	20050915	JP 2003-583993	20030401

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PRAI US 2002-370553P P 20020405
WO 2003-US9800 W 20030401
OS MARPAT 139:337785
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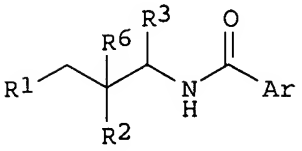

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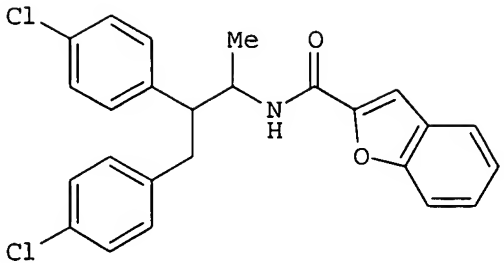


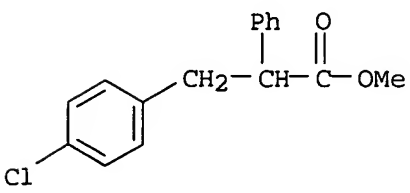
II

AB Title compds. I [wherein R1 = (un)substituted alkyl, (hetero)cycloalkyl, or (hetero)aryl; R2 = (un)substituted (hetero)cycloalkyl, (hetero)aryl, ORd, NRcRd, or CO2Rd; R3 = H or (un)substituted alkyl; R6 = H, halo, CN, NRcRd, or (un)substituted alkyl, alkenyl, or alkynyl; Ar = (un)substituted (hetero)aryl; Rc and Rd = independently H or (un)substituted alkyl, alkenyl, alkynyl, (hetero)cycloalkyl(alkyl), or (hetero)aryl(alkyl); or NRcRd = (un)substituted heterocyclyl; or two ORc groups together with the atoms to which they are attached = (un)substituted heterocyclyl; with provisos; and pharmaceutically acceptable salts thereof] were prepared by conventional and automated synthesis methods as antagonists and/or inverse agonists of the cannabinoid-1 (CB1) receptor (no data). For example, 2,3-bis(4-chlorophenyl)-1-methylpropylamine•HCl was acylated with 2-benzofurancarboxylic acid in the presence of PyBop and TEA in CH2Cl2 to give the desired amide II. I and their pharmaceutical compns. are useful as psychotropic drugs in the treatment of psychosis, memory deficits, cognitive disorders, migraine, neuropathy, neuroinflammatory disorders, including multiple sclerosis and Guillain-Barre syndrome, and the inflammatory sequelae of viral encephalitis, cerebral vascular accidents, and head trauma, anxiety disorders, stress, epilepsy, Parkinson's disease, movement disorders, and schizophrenia (no data). In addition, I and their pharmaceutical compns. are useful for the treatment of substance abuse disorders, the treatment of obesity or eating disorders, as well as the treatment of asthma, constipation, chronic intestinal pseudo-obstruction, and cirrhosis of the liver (no data).

IT **92907-23-8P**, 3-(4-Chlorophenyl)-2-phenylpropanoic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of substituted arylamides as CB1 receptor antagonists and/or inverse agonists for use as psychotropic drugs)

RN 92907-23-8 CAPLUS

CN Benzenepropanoic acid, 4-chloro-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



CAS ONLINE PRINTOUT

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:836767 CAPLUS
DN 139:337784
TI Preparation of substituted bicyclic arylamide cannabinoid-1 receptor antagonists and/or inverse agonists for use as psychotropic drugs
IN Castonguay, Laurie A.; Hagmann, William K.; Lin, Linus S.; Shah, Shrenik K.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 189 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003086288	A2	20031023	WO 2003-US10740	20030408
	WO 2003086288	A3	20040805		
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	US 2005203112	A1	20050915	US 2004-509584	20040929
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OS MARPAT 139:337784
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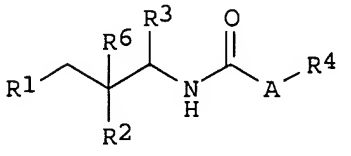

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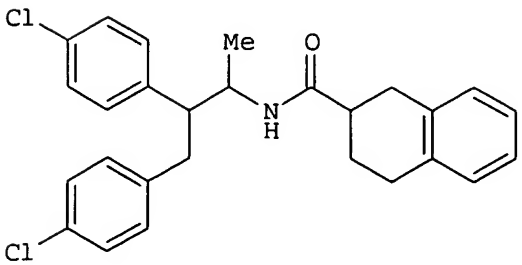


II

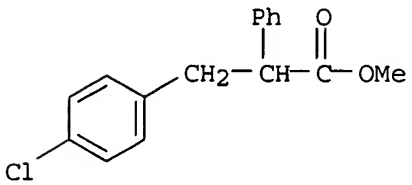
CAS ONLINE PRINTOUT

AB Title compds. I [wherein R1 = (un)substituted alkyl (hetero)cycloalkyl, or (hetero)aryl; R2 = (un)substituted (hetero)cycloalkyl, (hetero)aryl, ORd, NRcRd, or CO2Rd; R3 = (un)substituted (cyclo)alkyl, alkenyl, or alkynyl; R4 = H, ORc, CO2Rc, OCORc, OCO2Rc, OCONRdRe, NRdRe, NHCO2Rc, NRcSO2Rc, SO1-2Rc, or (un)substituted alkyl, alkenyl, alkynyl, or (hetero)aryl; R6 = H, halo, CN, NRcRd, or (un)substituted alkyl, alkenyl, or alkynyl; A = 3- to 8-membered (un)substituted monocyclic saturated ring incorporating the same C to which R4 is attached and optionally containing 1-2 heteroatoms, and to which a (hetero)aryl ring is fused, wherein said bicyclic ring is optionally fused to another (hetero)aryl ring to form a tricyclic ring; Rc and Rd = independently H or (un)substituted alkyl, alkenyl, alkynyl, (hetero)cycloalkyl(alkyl), or (hetero)aryl(alkyl); or NRcRd = (un)substituted heterocyclyl; or two ORc groups together with the atoms to which they are attached = (un)substituted heterocyclyl; Re = H, (cyclo)alkyl, alkenyl, alkynyl, (hetero)cycloalkyl(alkyl), or (hetero)aryl(alkyl); and pharmaceutically acceptable salts thereof] were prepared by conventional and automated synthesis methods as antagonists and/or inverse agonists of the cannabinoid-1 (CB1) receptor (no data). For example, 1,2,3,4-tetrahydro-2-naphthoic acid was converted to the acyl chloride using oxalyl chloride and DMF in CH2Cl2. Acylation of 2,3-bis(4-chlorophenyl)-1-methylpropylamine•HCl with the naphthoyl chloride in the presence of diisopropylethylamine in CH2Cl2 provided a diastereomeric mixture of amides II, which were separated on a silica gel column. I and their pharmaceutical compns. are useful as psychotropic drugs in the treatment of psychosis, memory deficits, cognitive disorders, migraine, neuropathy, neuroinflammatory disorders, including multiple sclerosis and Guillain-Barre syndrome, and the inflammatory sequelae of viral encephalitis, cerebral vascular accidents, and head trauma, anxiety disorders, stress, epilepsy, Parkinson's disease, movement disorders, and schizophrenia (no data). In addition, I and their pharmaceutical compns. are useful for the treatment of substance abuse disorders, the treatment of obesity or eating disorders, as well as the treatment of asthma, constipation, chronic intestinal pseudo-obstruction, and cirrhosis of the liver (no data). Novel compds. of the structural formula (I) are antagonists and/or inverse agonists of the Cannabinoid-1 (CB1) receptor and are useful in the treatment, prevention and suppression of diseases mediated by the CB1 receptor.

IT **92907-23-8P**, 3-(4-Chlorophenyl)-2-phenylpropanoic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of substituted bicyclic arylamide CB1 receptor antagonists and/or inverse agonists for use as psychotropic drugs)

RN 92907-23-8 CAPLUS

CN Benzenepropanoic acid, 4-chloro-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 6 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:796415 CAPLUS

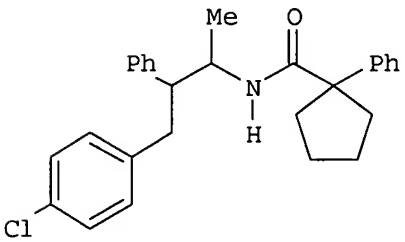
DN 139:307605

CAS ONLINE PRINTOUT

TI Preparation of spirocyclic carboxamides as cannabinoid receptor modulators
IN Hagmann, William K.; Lin, Linus S.; Shah, Shrenik K.; Goulet, Mark T.; Jewell, James P.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 224 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003082190	A2	20031009	WO 2003-US8722	20030321
	WO 2003082190	A3	20040219		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2479618	AA	20031009	CA 2003-2479618	20030321
	EP 1490043	A2	20041229	EP 2003-711667	20030321
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	JP 2005528366	T2	20050922	JP 2003-579733	20030321
	US 2005239828	A1	20051027	US 2004-507864	20040916
PRAI	US 2002-367655P	P	20020326		
	WO 2003-US8722	W	20030321		

OS MARPAT 139:307605
GI



I

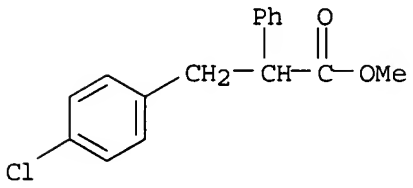
AB R1CH2CR2R3CHR4NHCOA [R1 = (un)substituted alkyl, cycloalkyl, heterocyclic, aryl; R2 = (un)substituted cycloalkyl, heterocyclic, aryl, OH, NH2, CO2H; R3 = H, (un)substituted alkyl, alkenyl, alkynyl, OH, NH2, halogen, CN; R4 = H, (un)substituted alkyl; A = (un)substituted 3-8-membered carbocyclic ring] were prepared and are antagonists and/or inverse agonists of the cannabinoid-1 (CB1) receptor, useful as psychotropic drugs in the treatment of psychosis, memory deficits, cognitive disorders, migraine, neuropathy, neuro-inflammatory disorders including multiple sclerosis and Guillain-Barre syndrome and the inflammatory sequelae of viral encephalitis, cerebral vascular accidents, and head trauma, anxiety disorders, stress, epilepsy, Parkinson's disease, movement disorders, and schizophrenia. The compds. are also useful for the treatment of substance abuse disorders, the treatment of obesity or eating disorders, as well as, the treatment of asthma, constipation, chronic intestinal pseudo-obstruction, and cirrhosis of the liver. Thus, PhCH2CO2Me was

treated with 4-ClC6H4CH2Br to give 4-ClC6H4CH2CHPhCO2Me which was hydrolyzed to the acid, converted to 4-ClC6H4CH2CHPhCONMeOMe, and treated with MeMgBr to give 4-ClC6H4CH2CHPhCOMe. This ketone was reduced to the alc., converted to the mesylate and then to the azide which was reduced to 4-ClC6H4CH2CHPhCHMeNH2.HCl. Treatment of this amine with phenylcyclopentanecarboxylic acid gave the amide I.

IT **92907-23-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of spirocyclic carboxamides as cannabinoid receptor modulators)

RN 92907-23-8 CAPLUS

CN Benzenepropanoic acid, 4-chloro-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 7 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:757469 CAPLUS
DN 139:276471
TI Preparation of substituted amides as antagonists and/or inverse agonists of the cannabinoid-1 receptor for therapy
IN Hagmann, William K.; Lin, Linus S.; Shah, Shrenik K.; Guthikonda, Ravindra N.; Qi, Hongbo; Chang, Linda L.; Liu, Ping; Armstrong, Helen M.; Jewell, James P.; Lanza, Thomas J., Jr.
PA Merck & Co., Inc., USA; et al.
SO PCT Int. Appl., 381 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003077847	A2	20030925	WO 2003-US7320	20030307
	WO 2003077847	A3	20041104		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2478183	AA	20030925	CA 2003-2478183	20030307
	EP 1496838	A2	20050119	EP 2003-714051	20030307
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	JP 2005519958	T2	20050707	JP 2003-575901	20030307
	US 2004058820	A1	20040325	US 2003-387265	20030312
	US 6972295	B2	20051206		
	US 2005234061	A1	20051020	US 2005-109076	20050419
PRAI	US 2002-363597P	P	20020312		

CAS ONLINE PRINTOUT

	US 2002-428351P	P	20021122
	WO 2003-US7320	W	20030307
	US 2003-387265	A3	20030312

OS MARPAT 139:276471

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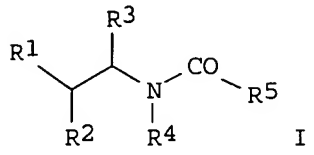
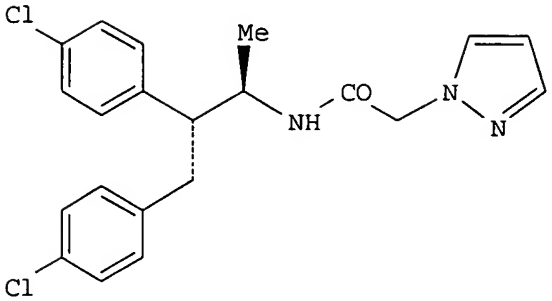


I

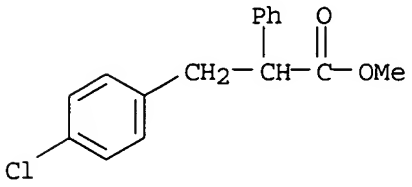


II

AB Novel compds. of the structural formula I (e.g. N-[2,3-bis(4-chlorophenyl)-1-methylpropyl]-2-(pyrazol-1-yl)acetamide trifluoroacetate (base shown as II with relative stereochem.); variables defined below) are antagonists and/or inverse agonists of the cannabinoid-1 (CB1) receptor (no data) and are useful in the treatment, prevention and suppression of diseases mediated by the CB1 receptor. The compds. of the present invention are useful as centrally acting drugs in the treatment of psychosis, memory deficits, cognitive disorders, migraine, neuropathy, neuro-inflammatory disorders including multiple sclerosis and Guillain-Barre syndrome and the inflammatory sequelae of viral encephalitis, cerebral vascular accidents, and head trauma, anxiety disorders, stress, epilepsy, Parkinson's disease, movement disorders, and schizophrenia. The compds. are also useful for the treatment of substance abuse disorders, the treatment of obesity or eating disorders, as well as the treatment of asthma, constipation, chronic intestinal pseudo-obstruction, and cirrhosis of the liver. Although the methods of preparation are not claimed, more than 120 example prepns. of intermediates and >480 example prepns./characterization data for a library of I are included. For I: R1 = C1-10-alkyl, C3-10cycloalkyl, C3-10-cycloalkyl-C1-4-alkyl, cycloheteroalkyl, cycloheteroalkyl-C1-4alkyl, aryl, aryl-C1-4-alkyl, heteroaryl, heteroaryl-C1-4-alkyl, -ORd, -NRcRd, -NRcC(O)Rd, -CO2Rd, and -C(O)NRcRd. R2 = C1-10alkyl, C3-10cycloalkyl-C1-4alkyl, cycloheteroalkyl, cycloheteroalkyl-C1-4alkyl, aryl, aryl-C1-4alkyl, aryloxy, arylthio, heteroaryl, and heteroaryl-C1-4alkyl; R3 = H, and C1-4alkyl; R4 = H, and C1-4alkyl; R5 = C1-10alkyl, C2-10alkenyl, C3-10-cycloalkyl-C1-4alkyl, cycloheteroalkyl-C1-4-alkyl, aryl-C1-4-alkyl, diaryl-C1-4alkyl, aryl-C1-4alkenyl, heteroaryl-C1-4alkyl, -ORd, and -NRcRd; addnl. details including provisos are given in the claims.

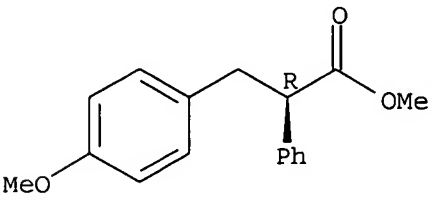
IT **92907-23-8P**, 3-(4-Chlorophenyl)-2-phenylpropanoic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of substituted amides as antagonists and/or inverse agonists of cannabinoid-1 receptor for therapy)
RN 92907-23-8 CAPLUS
CN Benzenepropanoic acid, 4-chloro-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 8 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:262921 CAPLUS
DN 139:85155
TI Intermolecular C-H activation at benzylic positions: synthesis of (+)-imperanene and (-)-α-conidendrin
AU Davies, Huw M. L.; Jin, Qihui
CS Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, NY, 14260-3000, USA
SO Tetrahedron: Asymmetry (2003), 14(7), 941-949
CODEN: TASYE3; ISSN: 0957-4166
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 139:85155
AB An efficient C-H activation of primary benzylic positions by means of rhodium carbenoid induced C-H insertions is described. This key step was used in concise syntheses of (+)-imperanene and (-)-α-conidendrin.
IT **553642-32-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of (+)-imperanene and (-)-α-conidendrin from a benzene derivative and a aryldiazoacetate via a rhodium carbenoid induced C-H insertion)
RN 553642-32-3 CAPLUS
CN Benzenepropanoic acid, 4-methoxy-α-phenyl-, methyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

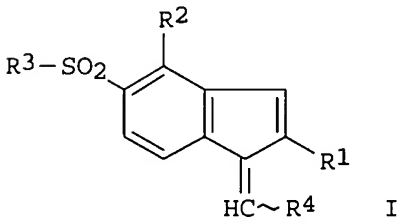
L13 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1999:9808 CAPLUS
DN 130:81284
TI Preparation of indene derivatives as COX 2 inhibitors

CAS ONLINE PRINTOUT

IN Matsuoka, Hiroharu; Maruyama, Noriaki; Kato, Yasuharu
PA Chugai Seiyaku Kabushiki Kaisha, Japan
SO PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9857924	A1	19981223	WO 1998-JP2611	19980615
	W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, GW, HU, ID, IL, IS, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	JP 11071342	A2	19990316	JP 1998-163372	19980611
	AU 9876749	A1	19990104	AU 1998-76749	19980615
PRAI	JP 1997-159598	A	19970617		
	WO 1998-JP2611	W	19980615		

OS MARPAT 130:81284
GI

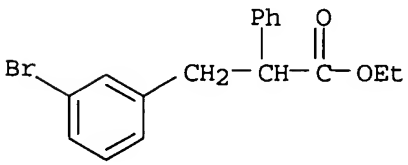


I

AB The title compds. I [R1 represents hydrogen etc.; R2 represents hydrogen etc.; R3 represents a C1-C3 linear or branched alkyl; and R4 represents an optionally substituted aryl etc.] are prepared The title compound (Z)-I [R1 = propyl; R2 = H; R3 = methyl; R4 = p-methoxyphenyl] in vitro showed IC50 values of 2 μM and 8 μM against COX-2 and COX-1, resp.

IT **218453-08-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indene derivs. as COX 2 inhibitors)

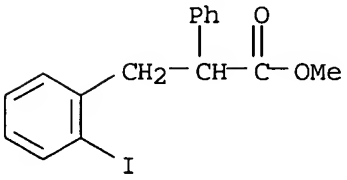
RN 218453-08-8 CAPLUS
CN Benzenepropanoic acid, 3-bromo-α-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAS ONLINE PRINTOUT

L13 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:785207 CAPLUS
DN 130:252002
TI Sandmeyer reactions. Part 4. An investigation into the cyclization modes of Pschorr phenanthrene synthesis
AU Hanson, Peter; Lovenich, P. Wilfried; Rowell, Simon C.; Walton, Paul H.; Timms, Allan W.
CS Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1999), (1), 49-64
CODEN: JCPKBH; ISSN: 0300-9580
PB Royal Society of Chemistry
DT Journal
LA English
AB Comparison of the cyclization regiochem. of the heterolysis and Cu-catalyzed homolysis of Me (E)-3-(2-diazoniophenyl)-2-(3-halophenyl)propenoate tetrafluoroborates indicates that the homolytic pathway involves direct closure of the 5-membered ring and not a 5-membered ring closure followed by ring expansion. From competition expts. in which homolytic cyclization of the corresponding non-halogenated compound was run against H abstraction from H3PO2, a cyclization rate constant kC = (3.0 ± 0.5) + 109 s-1 at ambient temperature was estimated which, when used in conjunction with a literature value for the homolytic phenylation of C6H6, allows evaluation of a statistically corrected effective molarity of 2 + 104 mol dm-3 for homolytic Pschorr phenanthrene closure. Regioselectivity considerations imply that, by contrast, heterolytic Pschorr phenanthrene closure exhibits unit effective molarity. A mechanistic rationale is presented to explain these patterns of behavior.
IT **221466-89-3P**
RL: BYP (Byproduct); PREP (Preparation)
(mechanism of Sandmeyer reaction in Pschorr phenanthrene synthesis)
RN 221466-89-3 CAPLUS
CN Benzenepropanoic acid, 2-iodo-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



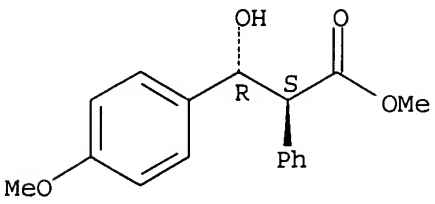
RE.CNT 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:23032 CAPLUS
DN 128:127797
TI Diastereoselective reactions of 1,1'-binaphthyl ester enolates with carbonyl electrophiles
AU Ahn, Mija; Tanaka, Kiyoshi; Fuji, Kaoru
CS Institute for Chemical Research, Kyoto University, Kyoto, 611, Japan
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1998), (2), 185-192
CODEN: JCPRB4; ISSN: 0300-922X
PB Royal Society of Chemistry
DT Journal
LA English

CAS ONLINE PRINTOUT

OS CASREACT 128:127797
AB Diastereoselectivity in the aldol and the conjugate addns. of 2'-hydroxy-1,1'-binaphthyl ester enolates with a variety of carbonyl electrophiles has been examined The ester enolate generated by BuLi reacts with several aldehydes to give the threo products preferentially with high diastereoselectivity and in good yield. Satisfactory diastereoselectivity has also been observed in the minor erythro derivs. A mechanistic interpretation of the results is made on the basis of the absolute stereochem. of the products.
IT **201746-39-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(diastereoselective reactions of 1,1'-binaphthyl ester enolates with carbonyl electrophiles)
RN 201746-39-6 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-4-methoxy-α-phenyl-, methyl ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

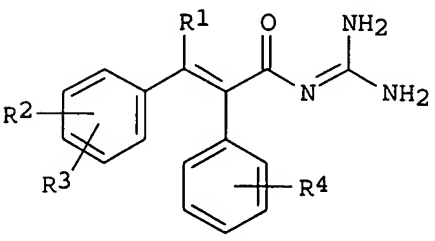


RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 12 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1997:280921 CAPLUS
DN 126:277281
TI Preparation of N-(2,3-diphenyl-2-propenoyl)guanidine derivatives as inhibitors of sodium/proton exchanger
IN Okazaki, Toshio; Kikuchi, Kazumi; Toyoshima, Hiroshi; Takanashi, Masahiro; Yanagisawa, Isao
PA Yamanouchi Pharma Co Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 09059245	A2	19970304	JP 1995-217869	19950825
PRAI JP 1995-217869		19950825		

OS MARPAT 126:277281
GI



I

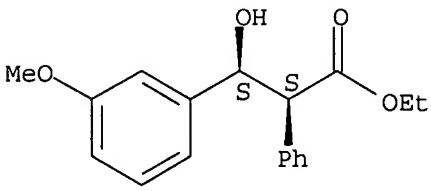
CAS ONLINE PRINTOUT

AB The title compds. [I; R1 = H, halo, lower alkyl; R2, R3, R4 = H, lower (halo)alkyl, lower alkenyl, lower alkynyl, cycloalkyl, lower alkoxy, lower alkoxy-lower alkyl, lower alkoxycarbonyl, CO2H, halo, NO2, cyano, NH2, mono- or di(lower alkyl)amino, lower alkanoyl, lower alkanoylamino, lower alkanoyloxy, OH, SH, lower alkylthio, lower alkylsulfonyl, mono- or di(lower alkyl)aminosulfonyl, etc.], which are useful for the treatment of hypertension, arrhythmia, and angina pectoris or as diagnostic agents for Na+/H+ exchanger-related hypertension, diabetes, and arteriosclerosis (no data), are prepared Thus, a mixture of 0.90 g (E)-3-(m-methoxyphenyl)-2-phenyl-2-propenoic acid (preparation given), 0.57 g 1,1'-carbonylbis(1H-imidazole), and 12 mL DMF was stirred at 50° for 30 min and ice-cooled, to which a solution of guanidine in DMF (preparation given), and the resulting mixture was stirred at room temperature for 3 h to give I (R1 = R3 = R4 = H, R2 = 3-MeO).

IT **188752-93-4P 188752-94-5P 188752-97-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-(diphenylpropenoyl)guanidine derivs. as inhibitors of sodium/proton exchanger)

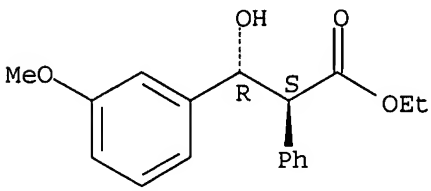
RN 188752-93-4 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-3-methoxy-α-phenyl-, ethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



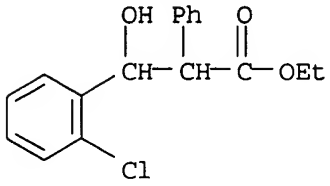
RN 188752-94-5 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-3-methoxy-α-phenyl-, ethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 188752-97-8 CAPLUS
CN Benzenepropanoic acid, 2-chloro-β-hydroxy-α-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

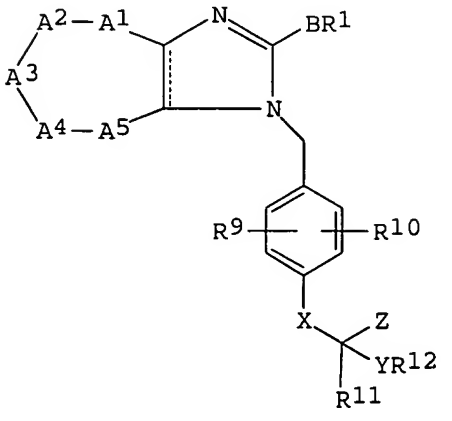
CAS ONLINE PRINTOUT



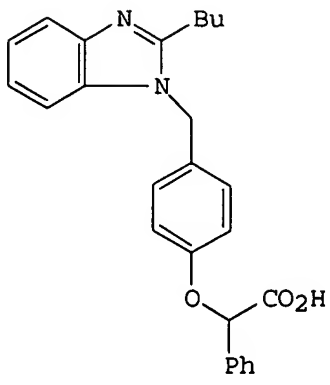
L13 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1991:656165 CAPLUS
DN 115:256165
TI Preparation of N-benzylated imidazopyridines and benzimidazoles as angiotensin II antagonists
IN Greenlee, William J.; Patchett, Arthur A.; Hangauer, David; Walsh, Thomas; Fitch, Kenneth J.; Rivero, Ralph A.; Dhanoa, Daljit S.
PA Merck and Co., Inc., USA
SO PCT Int. Appl., 401 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9111999	A1	19910822	WO 1991-US957	19910211
	W: CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
	CA 2075627	AA	19910814	CA 1991-2075627	19910211
	CA 2075637	AA	19910814	CA 1991-2075637	19910211
	EP 517812	A1	19921216	EP 1991-905733	19910211
	R: CH, DE, FR, GB, IT, LI, NL				
	JP 05504969	T2	19930729	JP 1991-505964	19910211
	US 5240938	A	19930831	US 1991-744557	19910813
	US 5264439	A	19931123	US 1991-744138	19910813
	US 5449682	A	19950912	US 1993-61975	19930517
PRAI	US 1990-479786	A	19900213		
	WO 1991-US957	W	19910211		
	US 1991-671551	B2	19910319		
	US 1991-671552	B2	19910319		
	US 1991-744557	A3	19910813		

OS MARPAT 115:256165
GI



I



II

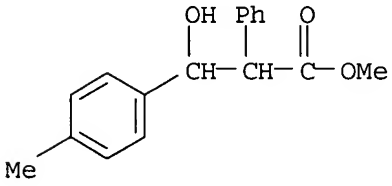
CAS ONLINE PRINTOUT

AB Title compds. [I; R1 = (substituted) alkyl, alkenyl, alkynyl, (hetero)aryl, perfluoroalkyl; R9, R10 = H, (cycloalkyl)alkyl, alkenyl, alkynyl, halo, alkoxy, perfluoroalkyl, (alkyl)cycloalkyl, aryl; adjacent R9R10 = CH:CHCH:CH; R11, R12 = H, (substituted) alkyl, aryl, arylalkyl, cycloalkyl; B = bond, SOn(CH2)s, O; n = 0-2; s = 0-5; X = O, SOn, imino, CH2O, CH2, CH2CH2, bond SOnCH2, etc.; Y = bond, SOn imino, CH2; Z = CO2H, alkoxycarbonyl, tetrazol-5-yl, arylsulfonylcarbamoyl, P(O)(OH)2, etc.; A1-A2-A3-A4-A5 = moieties to complete (substituted) benzene or heterocyclic (e.g., pyridine) rings], were prepared as antihypertensives, nootropics, anxiolytics, and antidepressants (no data). Thus, 2-butylbenzimidazole and 4-(PhCH2O)C6H4Cl were condensed to give 96% N-benzylated product, which was hydrogenolyzed (83%) followed by condensation with BrCHPhCO2Me (17%) and saponification (30%) to give title compound
II.

IT **137420-61-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as intermediate for angiotensin II antagonist)

RN 137420-61-2 CAPLUS

CN Benzenepropanoic acid, β-hydroxy-4-methyl-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 14 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1990:198049 CAPLUS

DN 112:198049

TI Preparation of some chromans substituted at the 3- or 4-position by an aryl or benzyl group by the rhodium-catalyzed intramolecular nucleophilic substitution of the corresponding 3-(2-fluorophenyl)propan-1-ols

AU Houghton, Roy P.; Shervington, Leroy A.

CS Coll. Cardiff, Univ. Wales, Cardiff, CF1 3TB, UK

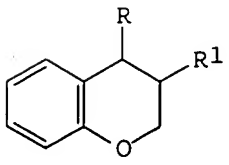
SO Journal of Chemical Research, Synopses (1989), (8), 239
CODEN: JRPSDC; ISSN: 0308-2342

DT Journal

LA English

OS CASREACT 112:198049

GI



I

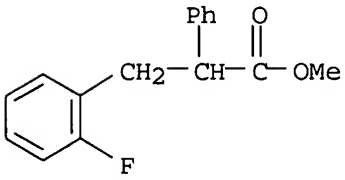
CAS ONLINE PRINTOUT

AB [Rh(η5-C5EtMe4)(η6-C6H6)][PF6]2 catalyzed the formation of chromans (I; R = H, CH2OH, Ph, 2-FC6H4, CH2Ph; R1 = Ph, 4-O2NC6H4, 4-MeOC6H4, CH2OH, H) from 2-FC6H4CHRCHR1CH2OH in MeNO2-Me2CO.

IT **126348-02-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 126348-02-5 CAPLUS

CN Benzenepropanoic acid, 2-fluoro-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 15 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1984:630289 CAPLUS

DN 101:230289

TI Studies on antifertility agents: part XLII - synthesis and antifertility study of 6-methoxy-3-phenyl-1-[p-(β-pyrrolidinoethoxy)phenyl]tetralin

AU Malik, Mangel S.; Rastogi, Shri Nivas

CS Med. Chem. Div., Cent. Drug Res. Inst., Lucknow, 226 001, India

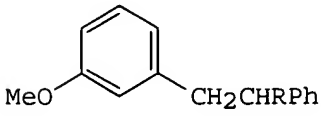
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(9), 834-8
CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

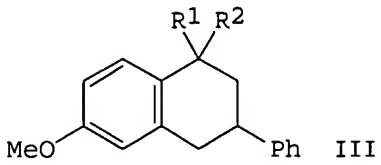
LA English

OS CASREACT 101:230289

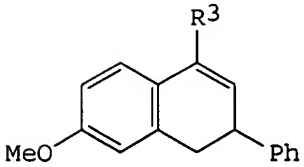
GI



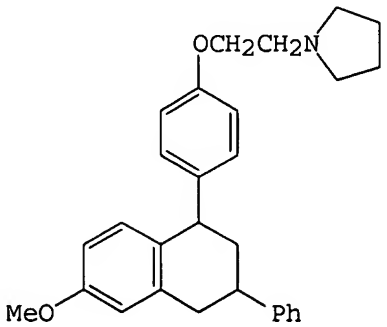
I



III



V



VI

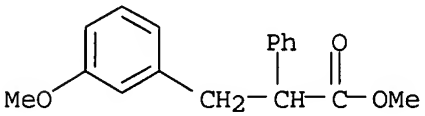
CAS ONLINE PRINTOUT

AB LiAlH4 reduction of ester I (R = MeO2C) gave the propanol I (R = HOCH2), which after treatment with p-TsCl and KCN gave butyronitrile I (R = NCCH2) (II). Alkaline hydrolysis of II gave acid I (R = HO2CCH2), which was cyclized on PCl5-SnCl4 to give tetralone derivative (III; R1R2 = O) (IV). KBH4 reduction of IV gave predominantly cis-tetrol (III; R1 = H, R2 = HO), which was condensed with PhOH-AlCl3 to give cis- and trans-III (R1 = H, R2 = 2- and 4-HOC6H4), and V (R3 = H). Reaction of Me2N(CH2)3MgCl with tetralone IV gave the propylamine V (R3 = Me2NCH2CH2CH2). Condensation of III (R1 = H, R2 = 4-HOC6H4) with N-(2-chloroethyl)pyrrolidine gave the title compound (VI).

IT **93273-50-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 93273-50-8 CAPLUS

CN Benzenepropanoic acid, 3-methoxy-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 16 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1984:209410 CAPLUS

DN 100:209410

TI β-Hydroxy esters

PA Mitsui Petrochemical Industries, Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 59013748	A2	19840124	JP 1982-123020	19820716
PRAI	JP 1982-123020		19820716		

AB Ten β-hydroxy esters were prepared by reaction of α-halo esters with Sn and carbonyl compds. in a polar solvent, followed by hydrolysis. Thus, PhCHBrCO2Et 243 and PhCHO 85 were added to Sn 131 mg in DMF at -45°, the mixture stirred overnight at -45°, and H2O added to give 78% HOCHPhCHPhCO2Et (84:16 erythro-threo).

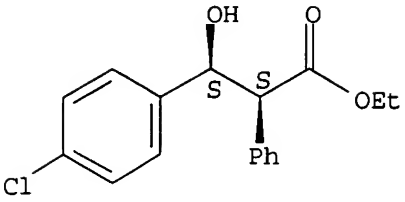
IT **81807-53-6P 81807-54-7P 81807-55-8P**
81807-56-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 81807-53-6 CAPLUS

CN Benzenepropanoic acid, 4-chloro-β-hydroxy-α-phenyl-, ethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

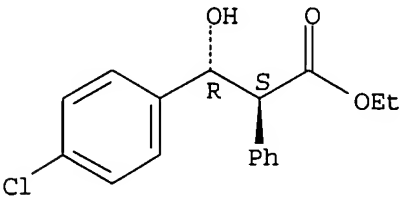
Relative stereochemistry.

CAS ONLINE PRINTOUT



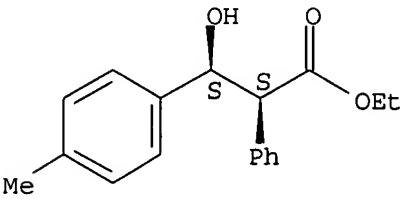
RN 81807-54-7 CAPLUS
CN Benzenepropanoic acid, 4-chloro-β-hydroxy-α-phenyl-, ethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



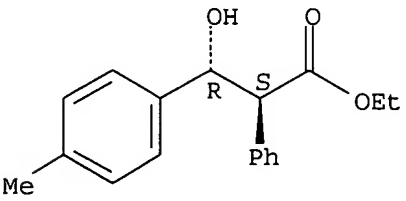
RN 81807-55-8 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-4-methyl-α-phenyl-, ethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 81807-56-9 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-4-methyl-α-phenyl-, ethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

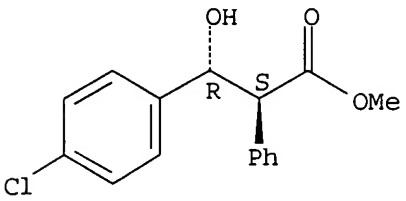


L13 ANSWER 17 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1982:581388 CAPLUS
DN 97:181388
TI Dehydrative decarboxylation of 2,3-disubstituted 3-hydroxycarboxylic acids with dimethylformamide acetals - apparent reaction course and preparative possibilities

CAS ONLINE PRINTOUT

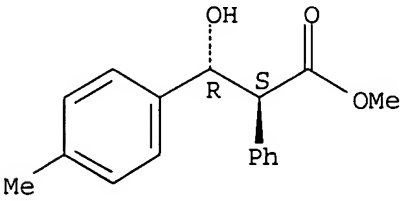
AU Mulzer, Johann; Bruentrup, Gisela
CS Inst. Org. Chem., Univ. Muenchen, Munich, D-8000/2, Fed. Rep. Ger.
SO Chemische Berichte (1982), 115(6), 2057-75
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA German
OS CASREACT 97:181388
AB Me2NCH(OMe)2 (I) converted threo-RCH(OH)CHR1CO2H (II; R = H, alkyl, vinyl, styryl, Ph, substituted Ph, 2-furyl, 2-thienyl; R1 = Me, Et, CHMe2, CMe3, Ph) to (E)- (III)/(Z)-RCH:CHR1 mixts. only when R = aryl or vinyl. The reaction had a marked E selectivity but was not a stereo-controlled olefin synthesis. If R = alkyl, the Me esters of II were obtained in the reaction. I reacted with erythro-II to give >98% sterically pure III. The fragmentation of zwitterionic intermediates was discussed.
IT **55006-65-0P 60079-78-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 55006-65-0 CAPLUS
CN Benzenepropanoic acid, 4-chloro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 60079-78-9 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-4-methyl-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L13 ANSWER 18 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1982:217397 CAPLUS
DN 96:217397
TI A new method for the synthesis of β-hydroxy esters by using metallic tin
AU Harada, Taira; Mukaiyama, Teruaki
CS Fac. Sci., Univ. Tokyo, Tokyo, 113, Japan
SO Chemistry Letters (1982), (2), 161-4
CODEN: CMLTAG; ISSN: 0366-7022
DT Journal
LA English
OS CASREACT 96:217397
AB Metallic Sn or activated metallic Sn, prepared by reduction of SnCl2 with

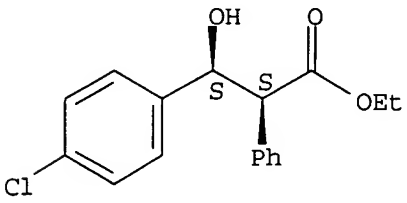
CAS ONLINE PRINTOUT

LiAlH4, smoothly reacts with α-halo esters to yield the Sn enolates, which in turn react with carbonyl compds. under mild conditions to give, after hydrolysis, β-hydroxy esters in high yields.

IT **81807-53-6P 81807-54-7P 81807-55-8P 81807-56-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

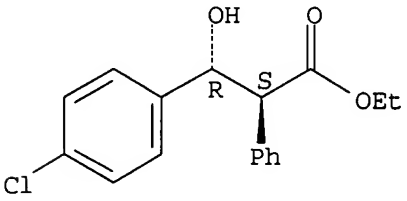
RN 81807-53-6 CAPLUS
CN Benzenepropanoic acid, 4-chloro-β-hydroxy-α-phenyl-, ethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



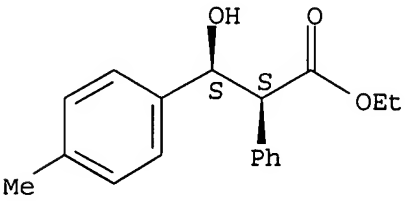
RN 81807-54-7 CAPLUS
CN Benzenepropanoic acid, 4-chloro-β-hydroxy-α-phenyl-, ethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 81807-55-8 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-4-methyl-α-phenyl-, ethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

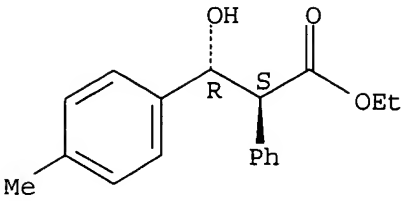
Relative stereochemistry.



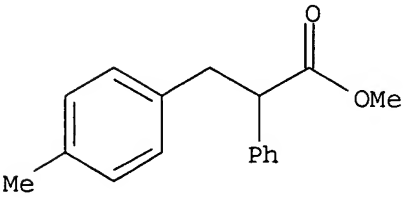
RN 81807-56-9 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-4-methyl-α-phenyl-, ethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

CAS ONLINE PRINTOUT



L13 ANSWER 19 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1979:419169 CAPLUS
DN 91:19169
TI Catalytic transfer reduction: scope and utility
AU Brieger, Gottfried; Nestrick, Terry J.; Fu, Tzuu-Heng
CS Dep. Chem., Oakland Univ., Rochester, MI, USA
SO Journal of Organic Chemistry (1979), 44(11), 1876-8
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
AB The Pd-catalyzed H transfer from organic donors to olefins, aromatic aldehydes, and ketones was studied. The intermediate benzyl alc. formed in the reduction of aromatic aldehydes can be trapped as the corresponding acetate. In the reduction of more complex ketones, ring opening occurs with cyclopropanes, and hydrogenolysis of aromatic halides also occurs. The relative effectiveness of a variety of donor compds. is also reported. Asym. induction during catalytic H transfer was explored with several systems, but no evidence of optical activity was found.
IT **69668-17-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 69668-17-3 CAPLUS
CN Benzenepropanoic acid, 4-methyl-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



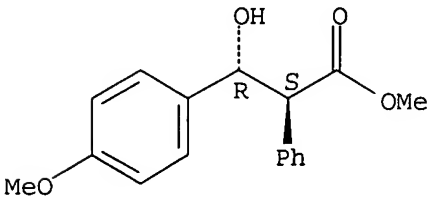
L13 ANSWER 20 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1978:529206 CAPLUS
DN 89:129206
TI Interaction of substituted benzaldehydes with methylphenylacetate during low-temperature Claisen reaction
AU Kirchev, N.; Krachanov, Kh.
CS Inst. Food Technol., Plovdiv, Bulg.
SO Doklady Bolgarskoi Akademii Nauk (1978), 31(1), 59-61
CODEN: DBANAD; ISSN: 0366-8681
DT Journal
LA English
AB Reaction of PhCH2CO2Me with RnC6H5-nCHO (Rn = H, 2-F, 2-Cl, 3-Cl, 2,6-Cl2, 3-Me, 4-MeO, etc.) in Et2O at -24° for 2 h in the presence of NaNH2 stopped at the aldol stage and gave eighteen RnC6H5-nCH(OH)CHPhCO2Me (I) in 31-85% yield, with threo/erythro ratio in the product varying from 96:4

to 69:31. There was no well-defined relation between the nature and position of the substituent and the yield of I.

IT **20445-41-4P 55006-62-7P 55006-63-8P 55006-64-9P 55006-65-0P 55006-67-2P 55006-68-3P 60079-78-9P 60079-81-4P 67710-01-4P 67710-04-7P 67710-05-8P 67710-06-9P 67722-11-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

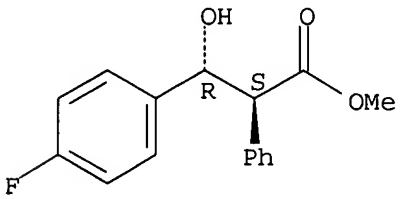
RN 20445-41-4 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-4-methoxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



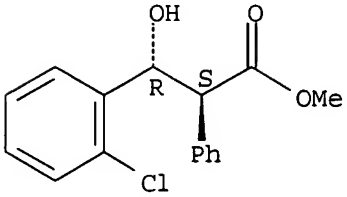
RN 55006-62-7 CAPLUS
CN Benzenepropanoic acid, 4-fluoro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 55006-63-8 CAPLUS
CN Benzenepropanoic acid, 2-chloro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

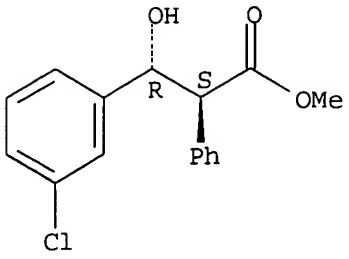
Relative stereochemistry.



RN 55006-64-9 CAPLUS
CN Benzenepropanoic acid, 3-chloro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

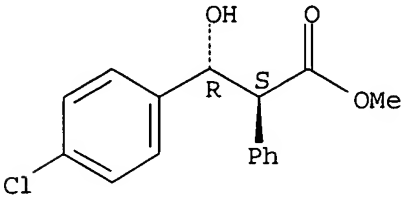
Relative stereochemistry.

CAS ONLINE PRINTOUT



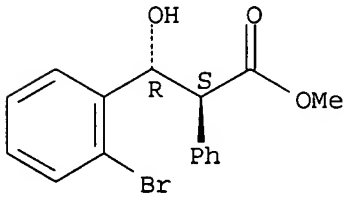
RN 55006-65-0 CAPLUS
CN Benzenepropanoic acid, 4-chloro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



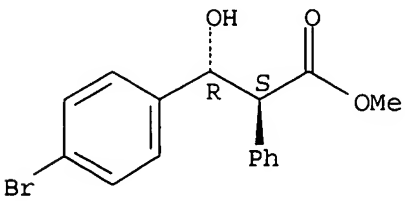
RN 55006-67-2 CAPLUS
CN Benzenepropanoic acid, 2-bromo-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 55006-68-3 CAPLUS
CN Benzenepropanoic acid, 4-bromo-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

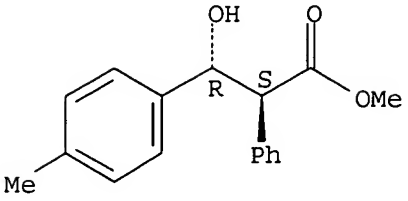
Relative stereochemistry.



RN 60079-78-9 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-4-methyl-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

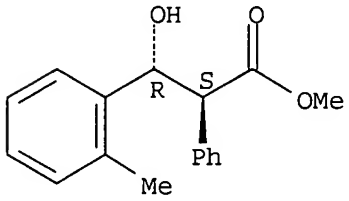
Relative stereochemistry.

CAS ONLINE PRINTOUT



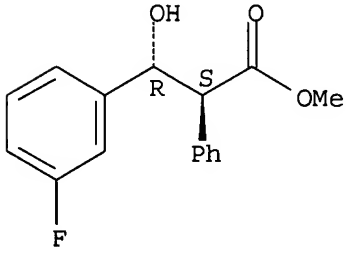
RN 60079-81-4 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-2-methyl-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



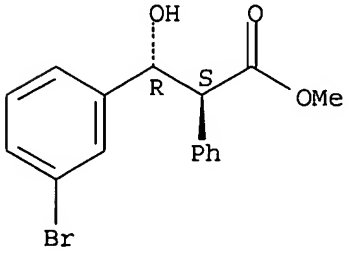
RN 67710-01-4 CAPLUS
CN Benzenepropanoic acid, 3-fluoro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 67710-04-7 CAPLUS
CN Benzenepropanoic acid, 3-bromo-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

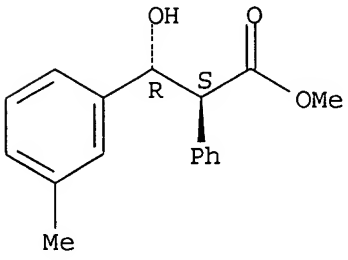
Relative stereochemistry.



RN 67710-05-8 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-3-methyl-α-phenyl-, methyl

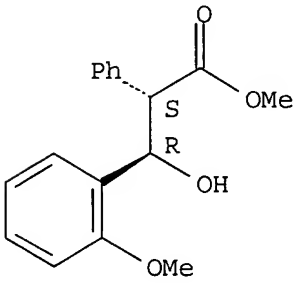
ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



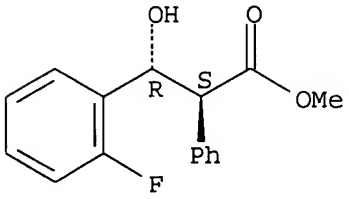
RN 67710-06-9 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-2-methoxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 67722-11-6 CAPLUS
CN Benzenepropanoic acid, 2-fluoro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



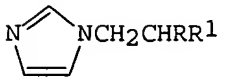
L13 ANSWER 21 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1977:72650 CAPLUS
DN 86:72650
TI 1-(β-Aryl-β-R-ethyl)imidazoles as antimicrobial agents
IN Heeres, Jan; Backx, Leo J. J.; Mostmans, Joseph H.
PA Janssen Pharmaceutica N. V., Belg.
SO U.S., 18 pp. Division of U.S. 3,927,017.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

CAS ONLINE PRINTOUT

PI	US 3991201	A	19761109	US 1975-578777	19750519
	US 3927017	A	19751216	US 1974-483587	19740627
PRAI	US 1974-483587	A3	19740627		

GI



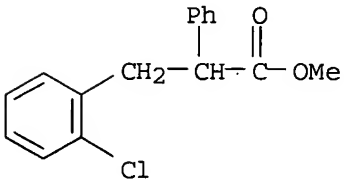
I

AB Arylethylimidazoles I (R = 4-FC6H4, 4-ClC6H4, 2-ClC6H4, 2,4-Cl2C6H3, 2,6-Cl2C6H3, Ph; R1 = C1-8 alkyl, allyl, 2-ClC6H4CH:CHCH2, chlorobenzyl, bromobenzyl, cyclohexyl, cyclopentyl, 4-MeOC6H4CH2, 4-MeC6H4CH2) (55 compds.) were prepared by treating RCH2CN with R1Br, hydrolyzing RR1CHCN, esterifying RR1CHCO2H, LiBH4 reduction of RR1CHCO2Me, treatment of RR1CHCH2OH with MeSO3H, and treatment of RR1CHCH2O3SMe with imidazole.

IT **59667-05-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 59667-05-9 CAPLUS

CN Benzenepropanoic acid, 2-chloro-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 22 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1976:477455 CAPLUS

DN 85:77455

TI Effect of substituents on the stereochemistry of the Reformatskii reaction

AU Mladenova, M.; Blagoev, B.; Kurtev, B.

CS Inst. Org. Chem., Sofia, Bulg.

SO Doklady Bolgarskoi Akademii Nauk (1975), 28(12), 1633-6
CODEN: DBANAD; ISSN: 0366-8681

DT Journal

LA French

AB The Reformatskii reaction of RC6H4CHO (R = H, p-Me, o-Me, p-Cl, o-Cl, p-MeO) and 1-naphthaldehyde with p-R1C6H4CHBrCO2Me (R1 = Br, H) gave an .apprx.50:50 mixture of erythro- and threo-RC6H4CH(OH)CH(C6H4R1-p)CO2Me or the 1-naphthyl analog in Et2O. In (MeO)2CH2, the erythro isomer was slightly favored (.apprx.60:40); in Me2SO, the threo isomer was favored (.apprx.70:30). In Me2SO, p-R1C6H4CH(CO2Me)CH(CO2Me)C6H4R-p was also formed. The lack of substituent effects in the Reformatskii reaction was explained by a transition state resembling the starting materials.

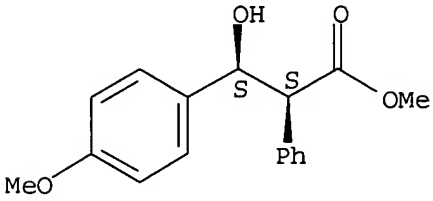
IT **20414-14-6P 20445-41-4P 55006-63-8P**
55006-65-0P 60079-78-9P 60079-79-0P
60079-80-3P 60079-81-4P 60079-82-5P
60079-83-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 20414-14-6 CAPLUS

CAS ONLINE PRINTOUT

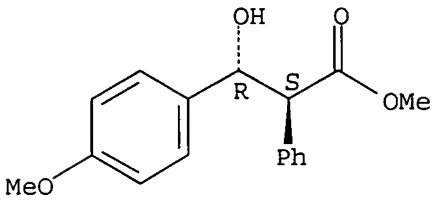
CN Benzenepropanoic acid, β-hydroxy-4-methoxy-α-phenyl-, methyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



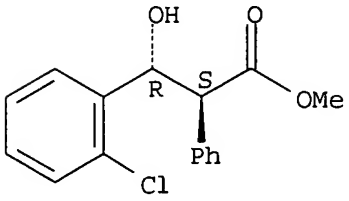
RN 20445-41-4 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-4-methoxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



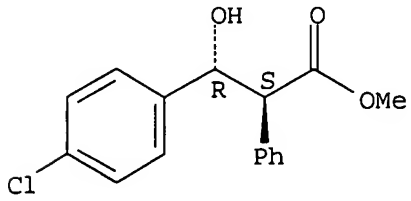
RN 55006-63-8 CAPLUS
CN Benzenepropanoic acid, 2-chloro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 55006-65-0 CAPLUS
CN Benzenepropanoic acid, 4-chloro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

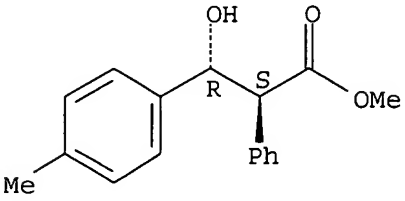
Relative stereochemistry.



RN 60079-78-9 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-4-methyl-α-phenyl-, methyl

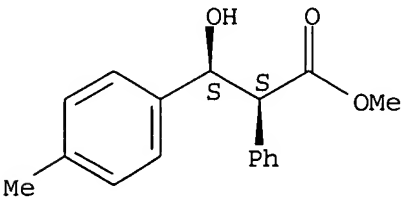
ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



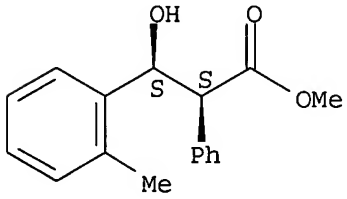
RN 60079-79-0 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-4-methyl-α-phenyl-, methyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



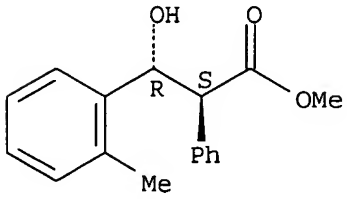
RN 60079-80-3 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-2-methyl-α-phenyl-, methyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 60079-81-4 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-2-methyl-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

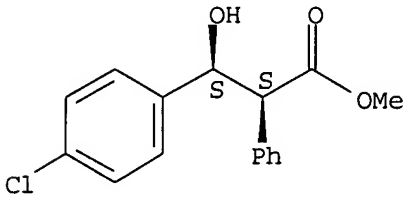
Relative stereochemistry.



RN 60079-82-5 CAPLUS
CN Benzenepropanoic acid, 4-chloro-β-hydroxy-α-phenyl-, methyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

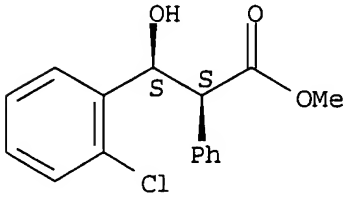
CAS ONLINE PRINTOUT

Relative stereochemistry.



RN 60079-83-6 CAPLUS
CN Benzenepropanoic acid, 2-chloro-β-hydroxy-α-phenyl-, methyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

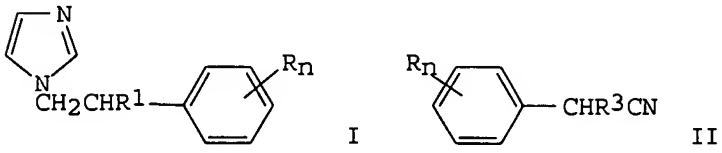
Relative stereochemistry.



L13 ANSWER 23 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1976:433007 CAPLUS
DN 85:33007
TI 1-(β-Aryl-β-R-ethyl)imidazoles
IN Heeres, Jan; Backx, Leo J. J.; Mostmans, Joseph H.
PA Janssen Pharmaceutica N. V., Belg.
SO U.S., 16 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3927017	A	19751216	US 1974-483587	19740627
	US 3991201	A	19761109	US 1975-578777	19750519
PRAI	US 1974-483587	A3	19740627		

GI



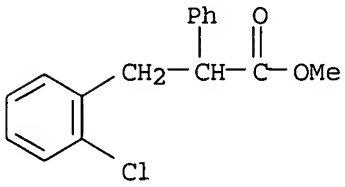
AB Imidazoles I [Rn = Cl, F, H, 2,4-, 2,6-Cl2; R1 = alkyl, allyl, cycloalkyl, CH2C6H5R2,CH2C6H4Cl2-2,4, CH2C6H4Cl2-2,6; R2 = Cl, Br, 4-Me, 4-MeO, CH2CH2Ph] (53 compds.), fungicides, bacteriostats, and bactericides at 0.1-100 γ/ml, were prepared by treating benzeneacetonitriles II (R3 = H) with halides R1X, hydrolyzing-esterifying II (R3 = R1) with HCl in MeOH or EtOH, reducing the ester RnC6H5-nCHR1CO2R4 (R4 = Me, Et) with NaBH4

over LiX in MeCN, mesylating the alc. RnC6H5-nCHR1CH2OH, and treating the methanesulfonate with imidazole.

IT **59667-05-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 59667-05-9 CAPLUS

CN Benzenepropanoic acid, 2-chloro-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 24 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1975:125008 CAPLUS

DN 82:125008

TI Application of the low temperature Claisen reaction for stereoselective synthesis of threo-3-aryl-3-hydroxy-2-phenylpropanoic acids and their methyl esters

AU Kurtev, B.; Kratchanov, Kh.; Kirchev, N.

CS Inst. Org. Chem., Sofia, Bulg.

SO Synthesis (1975), (2), 106-8
CODEN: SYNTBF; ISSN: 0039-7881

DT Journal

LA English

OS CASREACT 82:125008

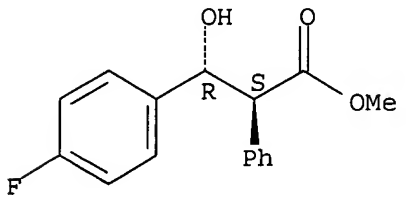
AB RCHO (R = Ph, 4-FC6H4, 2-, 3-, 4-ClC6H4, 2,6-Cl2C6H3, 2- and 4-BrC6H4) condensed with PhCH2CO2R1 (R1 = Me, CMe3) at -24° in Et2O or (Me2CH)2O containing NaNH2 gave threo-HOCHRCHPhCO2R1 (I) in 40-85% yield from the solid phase of the reaction mixture; I (R = Ph, R1 = CM3) was hydrolyzed to I (R = Ph, R1 = H) in 93% yield by heating with CF3CO2H. The I yield was lower and the erythro-threo ratio was higher in different solvents or with NaOEt instead of NaNH2.

IT **55006-62-7P 55006-63-8P 55006-64-9P**
55006-65-0P 55006-67-2P 55006-68-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 55006-62-7 CAPLUS

CN Benzenepropanoic acid, 4-fluoro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

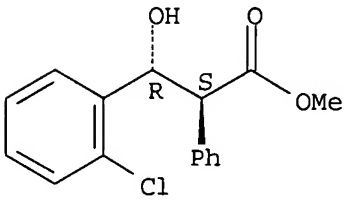


RN 55006-63-8 CAPLUS

CN Benzenepropanoic acid, 2-chloro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

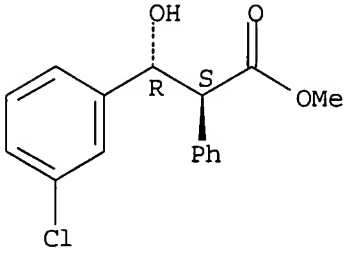
CAS ONLINE PRINTOUT

Relative stereochemistry.



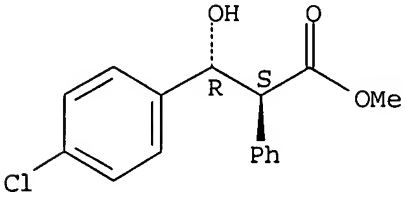
RN 55006-64-9 CAPLUS
CN Benzenepropanoic acid, 3-chloro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



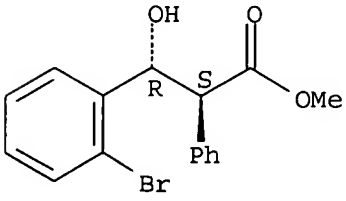
RN 55006-65-0 CAPLUS
CN Benzenepropanoic acid, 4-chloro-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 55006-67-2 CAPLUS
CN Benzenepropanoic acid, 2-bromo-β-hydroxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

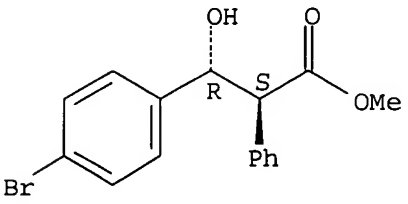


RN 55006-68-3 CAPLUS
CN Benzenepropanoic acid, 4-bromo-β-hydroxy-α-phenyl-, methyl

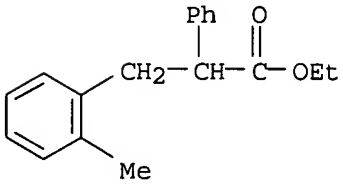
CAS ONLINE PRINTOUT

ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L13 ANSWER 25 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1974:477571 CAPLUS
DN 81:77571
TI Regiospecificity of methylation of unsymmetrical stilbenes by (methylsulfinyl)methanide
AU James, Brian G.; Pattenden, Gerald
CS Dep. Chem., Univ. Coll., Cardiff, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1974), (10), 1195-204
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
AB (E)-2-MeC6H4CH:CHPh with MeS(O)C-H2 for 2 min gave .apprx.50% (E)-2-MeC6H4CH:CMePh (I) and 2-MeC6H4CH [CH2S(O)Me]CH2Ph (II). Reaction for 2 hr gave a mixture of (E)(III) and (Z)-2-MeC6H4CMe:CHPh (IV) and 2-MeC6H4CH2-CHPh(CH2)2S(O)Me. The reactions of I, its Z-isomer, II, III, IV, and 2-MeC6H4CH2CHPhCH2S(O)Me with MeS(O)C-H2 are described. The mechanism and apparent regiospecificity of methylation by MeS(O)C-H2 are explained.
IT **53423-30-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 53423-30-6 CAPLUS
CN Benzenepropanoic acid, 2-methyl-α-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 26 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1974:107684 CAPLUS
DN 80:107684
TI Complex metal hydride reduction of carbon-carbon unsaturation. I. Sodium borohydride reduction of α-phenylcinnamates and related systems
AU Schauble, J. Herman; Walter, Gerald J.; Morin, J. Guy
CS USA
SO Journal of Organic Chemistry (1974), 39(6), 755-60
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English

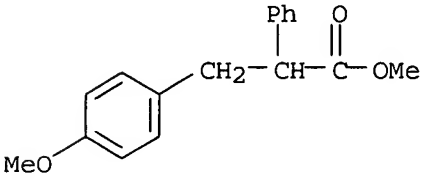
CAS ONLINE PRINTOUT

AB Competitive rates of NaBH4 reduction for two sets of Me α-phenyl-trans-cinnamates, para-substituted in the α and β rings, resp., correlate linearly with Hammett substituent consts. The similarity in ρα (1.74) and ρβ (1.44) indicates that the transition state for hydride transfer occurs before significant change in geometry of the α,β-unsatd. carbonyl system occurs. Competitive rate studies for Me α-(para-substituted phenyl)acrylates and Me α-phenyl-cis- and -trans-crotonates are corroborated by the data obtained for the cinnamates.

IT **5448-41-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 5448-41-9 CAPLUS

CN Benzenepropanoic acid, 4-methoxy-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 27 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1969:490560 CAPLUS

DN 71:90560

TI Kinetics of the decarboxylative dehydration of β-anisyl-β-hydroxy-α-phenylpropionic acid

AU Noyce, Donald S.; McGoran, Ernest C.

CS Univ. of California, Berkeley, CA, USA

SO Journal of Organic Chemistry (1969), 34(9), 2558-61
CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

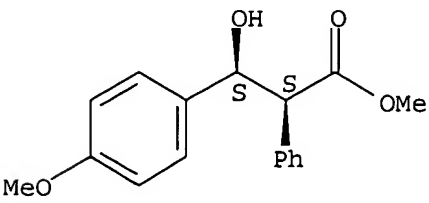
AB The decarboxylative dehydrations of erythro- and threo-β-anisyl-β-hydroxy-α-phenylpropionic acids proceed at different rates in dilute aqueous H2SO4. Both stereoisomers give trans-4-methoxystilbene. The diastereoisomers are interconverted at a rate which is lower than decarboxylation in dilute H2SO4, but at a rate more rapid than decarboxylation in more acidic medium. These facts are interpreted in terms of generation of a dipolar ion which loses CO2 more rapidly than it reacts with water.

IT **20414-14-6P 20445-41-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 20414-14-6 CAPLUS

CN Benzenepropanoic acid, β-hydroxy-4-methoxy-α-phenyl-, methyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

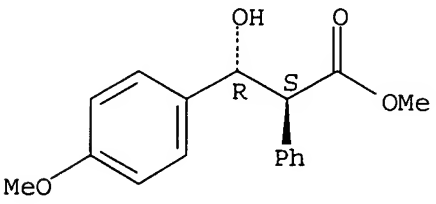
Relative stereochemistry.



CAS ONLINE PRINTOUT

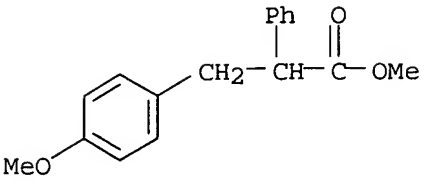
RN 20445-41-4 CAPLUS
CN Benzenepropanoic acid, β-hydroxy-4-methoxy-α-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

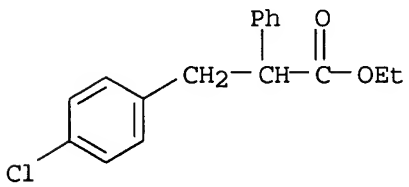


L13 ANSWER 28 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1968:486787 CAPLUS
DN 69:86787
TI Heterocyclic compounds. Synthesis of α-phenyl-β-(4-methoxyphenyl)propionic esters; isomers of 1,2,5-trimethyl- and 1-allyl-2,5-dimethyl-4-piperiodols
AU Sharifkanov, A. Sh.; Yusupov, S. A.; Starodubova, G.
CS USSR
SO Sb. Statei Aspir. Soiskatelei, Min. Vyssh. Sredn. Spets. Obrazov. Kaz. SSR, Khim. Khim. Tekhnol. (1966), 5, 164-7
From: Ref. Zh., Khim. 1967, Abstr. No. 22Zh330
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB α-Phenyl-β-(4-methoxyphenyl)propionic esters of α-isomers of 1,2,5-trimethyl- (I) and 1-allyl-2,5-dimethyl-4-piperidinols (II) were synthesized. α-Phenyl-β-(4-hydroxyphenyl)propionic acid (III) (12.1 g.) is added to a solution of 4 g. NaOH in 40 ml. of H2O while cooling, and after 1 hr., 13.8 g. Me2SO4 is added. The solution is heated 3 hrs. in a bath at .apprx.100° to give 80% Me α-phenyl-β-(4-methoxyphenyl)propionate (IV), b3 188-90°, m. 56-7°. III in ether with CH2N2 gives 88.2% IV. A solution of 7.05 g. KOH in 126 ml. MeOH is added to a solution of 17 g. IV in 50 ml. MeOH and the mixture heated 1.5 hrs. at 60° to give 98.1% free acid (V), m. 121-2° (1:2 MeOH-H2O). A mixture of 16 g. V and 14.88 g. SOCl2 is heated 1 hr. at 60° and 2 hrs. at 100-5° to give the acid chloride, m. 54-5°. A mixture of 2.14 g. of the α-isomer of 1,2,5-trimethyl-4-piperidinol, 8.1 g. of the acid chloride, 0.1 g. Mg shavings, and 10 ml. dioxane is heated for 10 hrs. at 110-15° to give 54.8% VI.HCl, m. 61-2°. Under similar conditions, 2.5 g. of the α-isomer of VII in 10 ml. dioxane, 0.1 g. Mg, and 8 g. of the acid chloride of V gave 87.3% VII.HCl, m. 49-51°. The acid chloride (10.4 g.) of VI is added to a solution of 3.4 g. II in 8 ml. pyridine and the mixture heated 12 hrs. at 125-30° to yield VII, 80.05%, VII, n13.5D 1.5510.
IT **5448-41-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 5448-41-9 CAPLUS
CN Benzenepropanoic acid, 4-methoxy-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)

CAS ONLINE PRINTOUT



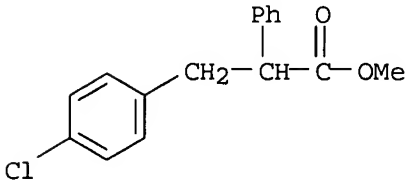
L13 ANSWER 29 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1965:462680 CAPLUS
DN 63:62680
OREF 63:11419b-d
TI Alkylations of phenylacetic, α-alkylphenylacetic, and diphenyl-acetic esters by means of sodamide and sodium hydride
AU Kenyon, William G.; Kaiser, Edwin M.; Hauser, Charles R.
CS Duke Univ., Durham, NC
SO Journal of Organic Chemistry (1965), 30(9), 2937-42
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 63:62680
AB Various alkylations of Et and tert-Bu phenyl-acetates with alkyl halides and further alkylations of the resulting α-alkylphenylacetic esters were effected by means of sodamide in liquid ammonia. The method was successful even with p-chloro- and p-methoxyphenylacetic esters and with p-chlorobenzyl chloride. Typical alkylations were also effected by means of NaH in refluxing monoglyme. Sodamide was preferable for monoalkylations of Et or tert-Bu phenylacetates, but the 2 reagents were about equally effective for further alkylations of α-alkylphenylacetic esters. NaH was better for dialkylation of Et phenylacetate with the same halide in a single operation. The present methods were superior to earlier methods. Also the present methods appear useful for the synthesis of certain mono- and dialkylarylacetic acids, which were obtained on hydrolysis of the alkylated esters. Et diphenylacetate was alkylated with certain halides by means of sodamide in liquid ammonia.
IT **3152-55-4**, Propionic acid, 3-(p-chlorophenyl)-2-phenyl-, ethyl ester
(preparation of)
RN 3152-55-4 CAPLUS
CN Propionic acid, 3-(p-chlorophenyl)-2-phenyl-, ethyl ester (7CI, 8CI) (CA INDEX NAME)



L13 ANSWER 30 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1963:408668 CAPLUS
DN 59:8668
OREF 59:1523d-e
TI Reactions of active methylene compounds in pyridine solution. V. α-Hydroperoxy esters

CAS ONLINE PRINTOUT

AU Avramoff, M.; Sprinzak, Y.
CS Weizmann Inst. Sci., Rehovoth, Israel
SO Journal of the American Chemical Society (1963), 85, 1655-7
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
OS CASREACT 59:8668
AB cf. CA 55, 19858h. Base-catalyzed autoxidn. of esters of diarylacetic acids and 2,3-diarylpropionic acids affords α-hydroperoxy esters RCAr(OOH)CO2R', a novel type of hydroperoxides, along with α-hydroxy esters and ketones. The formation of the latter two types of compds. is explained in terms of reduction and decomposition of the hydroperoxy esters.
IT **92907-23-8**, Propionic acid, 3-(p-chlorophenyl)-2-phenyl-, methyl ester
(preparation of)
RN 92907-23-8 CAPLUS
CN Benzenepropanoic acid, 4-chloro-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 31 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1959:44989 CAPLUS
DN 53:44989
OREF 53:8065f-i,8066a-b
TI Preparation of substituted α,β-diphenylacrylic acids and related derivatives
AU Alexander, B. H.; Barthel, W. F.
CS U.S. Dept. of Agr., Beltsville, MD
SO Journal of Organic Chemistry (1958), 23, 389-91
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA Unavailable
OS CASREACT 53:44989
AB cf. C.A. 52, 9022a. Et β-(3,4-methylenedioxyphenyl)-α-phenylacrylate, RR1C6H3CH:CPhCO2R2 (I) (RR1 = 3,4-CH2O2, R2 = OEt) (II) (loc. cit.), was shown to be an excellent synergist for pyrethrum when tested against lice. Related compounds were prepared The reported acrylic acids are trans compds. as indicated by m.p. data. p-MeOC6H4CHO and PhCH2CO2H condensed as previously described for the methylenedioxyphenyl compds. (loc. cit.), the crude acid (43%) stirred rapidly with 50% alc. at 50°, and the solution cooled gave p-MeOC6H4CH(OH)CHPhCO2H (III), m. 136-8° (decomposition). III (89 g.) and 50 g. anhydrous NaOAc stirred 4 hrs. in 200 ml. Ac2O on a steam bath, the hot mixture poured onto 1 kg. cracked ice with stirring, kept overnight, and the water-washed precipitate recrystd. (95% alc.) yielded 75% p-MeOC6H4CH:CHPh, m. 135-6°. Similar decarboxylation of the corresponding 3,4-CH2O2C6H3CH(OH)CHPhCO2H gave 97% I (RR1 = 3,4-CH2O2, R2 = OH) and not 3,4-CH2O2C6H3CH: CHPh (IV). Crude α-benzylpiperonyl alc. chrysanthemumate [cf. U.S. Dept. Agriculture ARS-33-42, Procedures C and E (1957)] distilled at 145-80°/0.2 mm. in a short-path still gave a quant. yield of IV, m. 93-4° (95% alc.). MeO analogs of I were prepared as for II. I (R = H, R1 = o-MeO, R2 = OH) (V), m. 185-7° (3:1 alc.-H2O),

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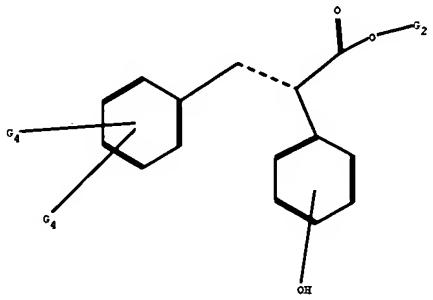

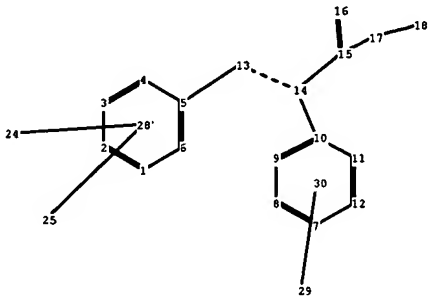

chain nodes :
13 14 15 16 17 18 24 25 29
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
5-13 10-14 13-14 14-15 15-16 15-17 17-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
13-14 15-16 15-17 17-18
exact bonds :
5-13 10-14 14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,OH

G2:CH3,Et,n-Pr,i-Pr

G3:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,X

G4:MeO,EtO,n-PrO,i-PrO

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS
18:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS